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# Mean-field calculation including proton-neutron mixing in atomic nuclei —toward proton-neutron pairing—

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◆ “Nuclear DFT (density functional theory) with proton-neutron pairing and its application”  
(e.g. GT transition in r-process)

- Proton-neutron (p-n) pairing: Goodman, Adv. Nucl. Phys.11, (1979) 293.

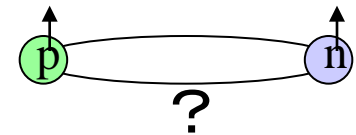
Pairing between protons and neutrons (isoscalar  $T=0$  and isovector  $T=1$ )

Related (?) physics:

Wigner energy,  $\beta$  decays, interplay between  $T=0$  and  $T=1$  states in  $N=Z$  nuclei, isospin mixing and mirror symmetry breaking,  $\alpha$  decay and  $\alpha$  clustering, moments of inertia, deformation properties, etc.

Perlinska et al, PRC 69, 014316(2004)

For a review on  $p$ - $n$  pairing, see A. Afanasjev, arXiv:1205.2134



- Proton-neutron mixing:

Quasiparticles are mixtures of protons and neutrons

Density functionals with an arbitrary mixing between protons and neutrons

$$\rho_{\tau}(\alpha, \beta) = \langle \Psi | c_{\alpha, \tau}^{\dagger} c_{\beta, \tau} | \Psi \rangle \longrightarrow \rho_{\tau \tau'}(\alpha, \beta) = \langle \Psi | c_{\alpha, \tau}^{\dagger} c_{\beta, \tau'} | \Psi \rangle$$

$\tau = p, n$   $\tau, \tau' = p, n$

As a first step, we consider p-n mixing at the Hartree-Fock level without pairing.

# Hartree-Fock calculation including proton-neutron mixing

- Extension of the single particle states

$$\begin{aligned}
 |\psi_{i,n}\rangle &= \sum_{\alpha} a_{i,\alpha}^{(n)} |\alpha, n\rangle \\
 |\psi_{j,p}\rangle &= \sum_{\alpha} a_{j,\alpha}^{(p)} |\alpha, p\rangle
 \end{aligned}
 \longrightarrow
 \begin{aligned}
 |\psi_i\rangle &= \sum_{\alpha} a_{i,\alpha}^{(n)} |\alpha, n\rangle + \sum_{\beta} a_{i,\beta}^{(p)} |\beta, p\rangle
 \end{aligned}
 \quad i=1, \dots, A$$

- Extension of the density functional

$$E^{Skyrme}[\rho_n, \rho_p] \longrightarrow E^{Skyrme'}[\rho_0, \vec{\rho}]$$

isoscalar
isovector

**Invariant under rotation in isospin space**

Perlinska et al, PRC 69 , 014316(2004)

can be written in terms of  $\rho_0, \rho_3$

**not invariant under rotation in isospin space**

$$\begin{aligned}
 \rho_0 &= \rho_n + \rho_p & \rho_1 &= \rho_{np} + \rho_{pn} \\
 \rho_2 &= -i\rho_{np} + i\rho_{pn} \\
 \rho_3 &= \rho_n - \rho_p
 \end{aligned}$$

**Energy density functional is extended such that it becomes invariant under rotation in isospin space**

# Hartree-Fock calculation including proton-neutron mixing

- Extension of the single particle states

$$\begin{aligned}
 |\psi_{i,n}\rangle &= \sum_{\alpha} a_{i,\alpha}^{(n)} |\alpha, n\rangle \\
 |\psi_{j,p}\rangle &= \sum_{\alpha} a_{j,\alpha}^{(p)} |\alpha, p\rangle
 \end{aligned}
 \longrightarrow
 \begin{aligned}
 |\psi_i\rangle &= \sum_{\alpha} a_{i,\alpha}^{(n)} |\alpha, n\rangle + \sum_{\beta} a_{i,\beta}^{(p)} |\beta, p\rangle
 \end{aligned}
 \quad i=1, \dots, A$$

- Extension of the density functional

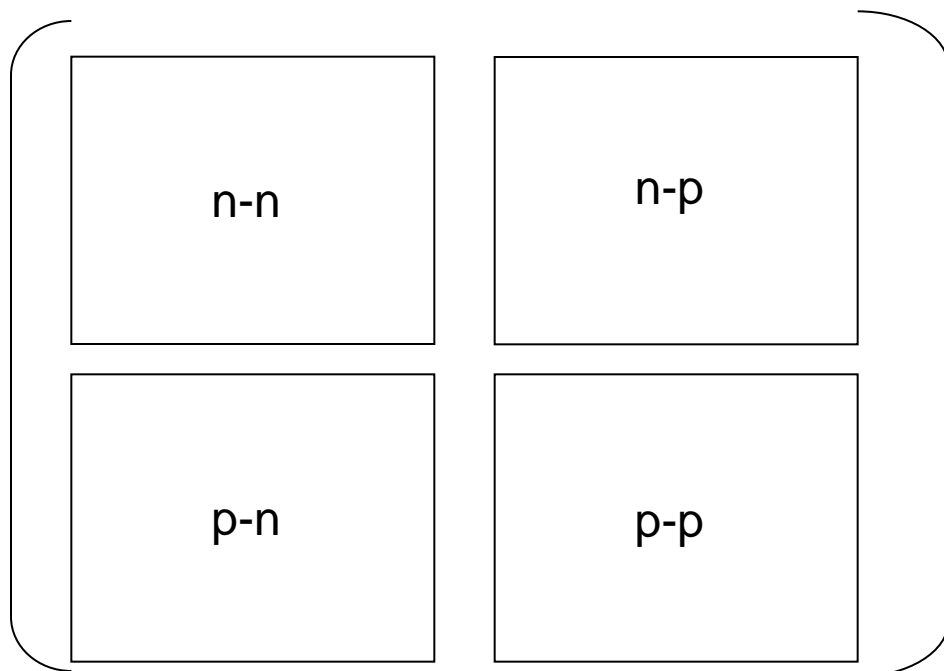
$$E^{Skyrme}[\rho_n, \rho_p] \longrightarrow E^{Skyrme'}[\rho_0, \vec{\rho}] \quad \text{Invariant under rotation in isospace}$$

isoscalar
isovector

Perlinska et al, PRC 69 , 014316(2004)

- p-n mixed Hartree-Fock Hamiltonian :

$$h_n, h_p \longrightarrow h_{mixed} =$$



Off-diagonal blocks are zero  
in the normal HF w/o p-n mixing

It is a hard task to develop a code from scratch ...

—————→ Use of an existing HFB code

## HFODD(1997-)

<http://www.fuw.edu.pl/~dobaczew/hfodd/hfodd.html>

J. Dobaczewski, J. Dudek, Comp. Phys. Comm 102 (1997) 166.  
J. Dobaczewski, J. Dudek, Comp. Phys. Comm. 102 (1997) 183.  
J. Dobaczewski, J. Dudek, Comp. Phys. Comm. 131 (2000) 164.  
J. Dobaczewski, P. Olbratowski, Comp. Phys. Comm. 158 (2004) 158.  
J. Dobaczewski, P. Olbratowski, Comp. Phys. Comm. 167 (2005) 214.  
J. Dobaczewski, et al., Comp. Phys. Comm. 180 (2009) 2391.  
J. Dobaczewski, et al., Comp. Phys. Comm. 183 (2012) 166.

- Skyrme energy density functional
- Hartree-Fock or Hartree-Fock-Bogoliubov
- No spatial & time-reversal symmetry restriction
- Harmonic-oscillator basis
- Multi-function (constrained HFB, cranking, angular mom. projection, isospin projection, finite temperature....)

# Road map

HFODD (Skyrme-HF(B) code)



Proton-neutron mixing at HF level

→ **Test calc. for A=14 and 48 nuclei**



Isospin projection with p-n mixing

to remove spurious isospin mixing



Proton-neutron pairing (T=1 & T=0)



QRPA with FAM, Isospin projection w/ p-n pairing, etc.

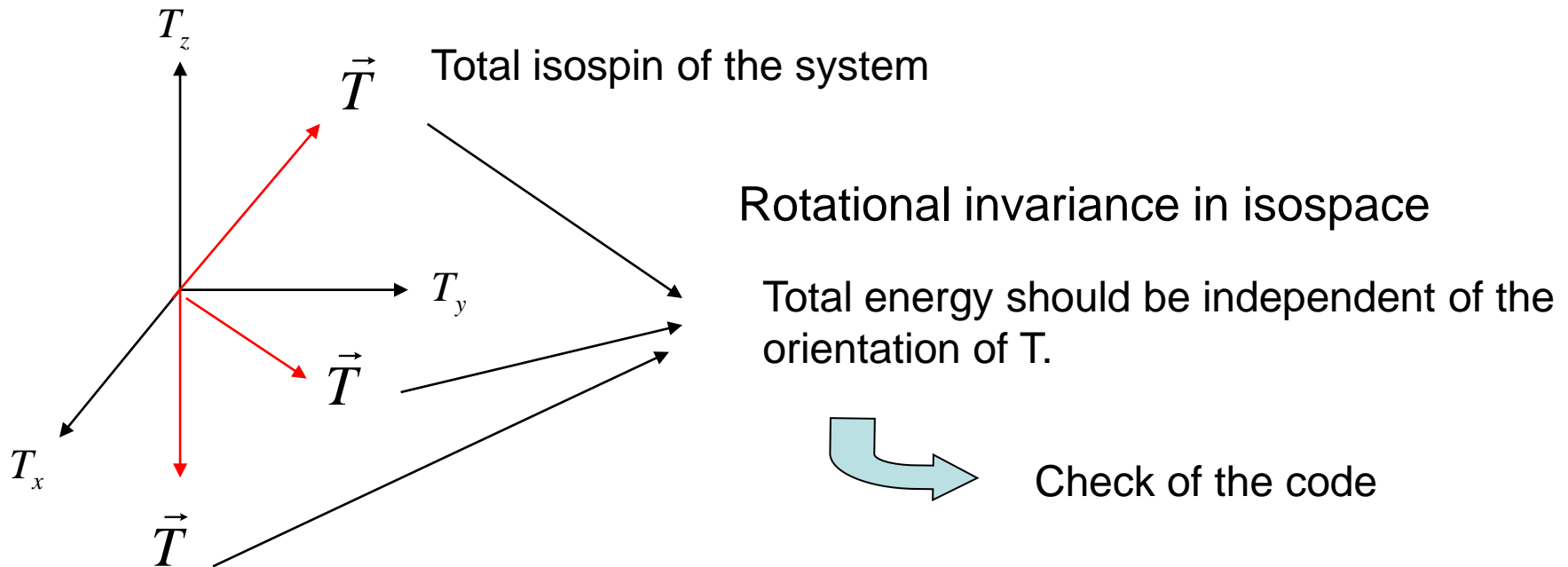
e.g. calc. of GT strengths of n-rich nuclei

## Test calculations for p-n mixing

### EDF with p-n mixing is correctly implemented?

w/o Coulomb force (and w/ equal proton and neutron masses)

$$\mathcal{H} = \mathcal{H}_{\text{kin}} + \mathcal{H}_{\text{Skyrme}} \quad \text{:invariant under rotation in isospin space}$$



How to control the isospin direction ?

# Isocranking calculation

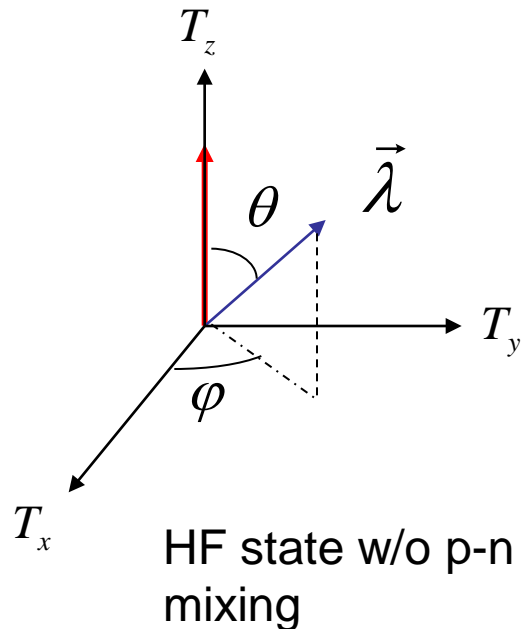
$$\hat{H}' = \hat{H} - \vec{\lambda} \cdot \vec{T} \quad \text{Isocranking term}$$

$\vec{\lambda}$  : Input frequency to control the isospin of the system

HF eq. solved by iterative diagonalization of MF Hamiltonian.

w/ p-n mixing and no Coulomb

Initial state: HF solution w/o p-n mixing (e.g.  $^{14}\text{C}(T_z=1, T_x=1)$ )

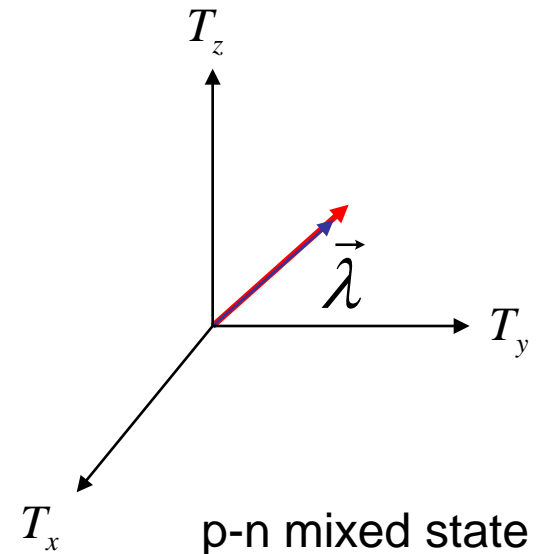


Determine s. t. proton and neutron Fermi energies become equal

$$-\vec{\lambda} \cdot \vec{T}$$

iteration

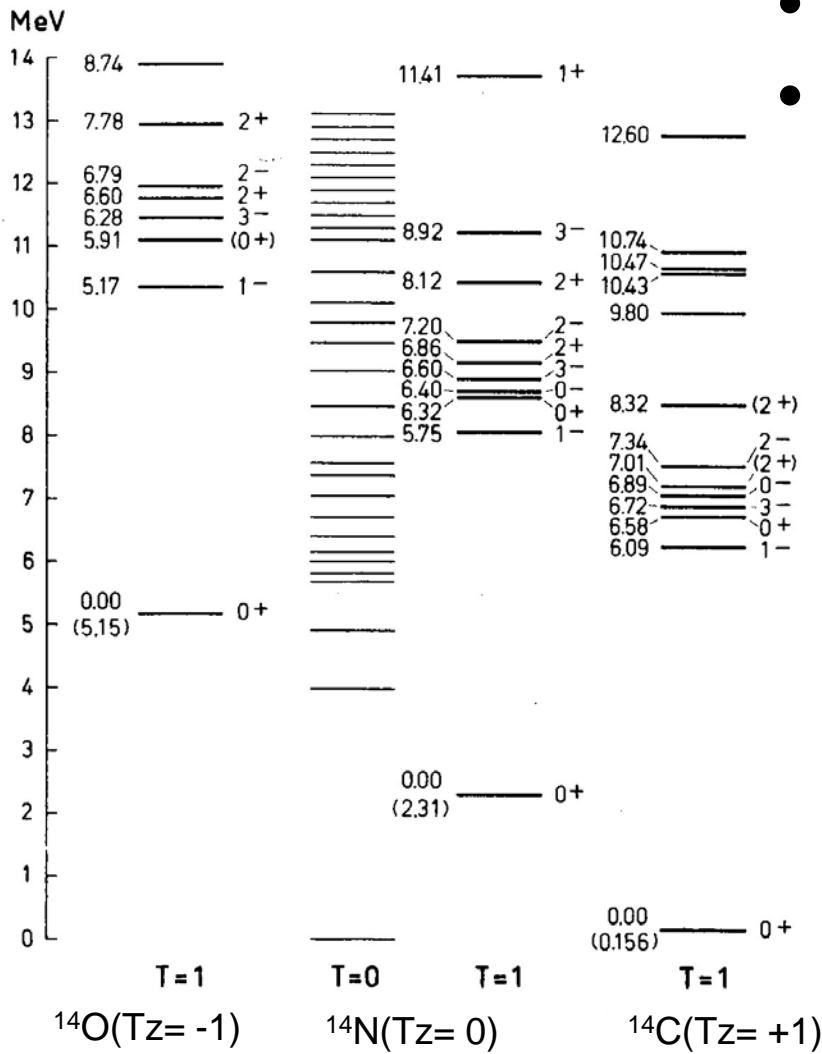
Final state



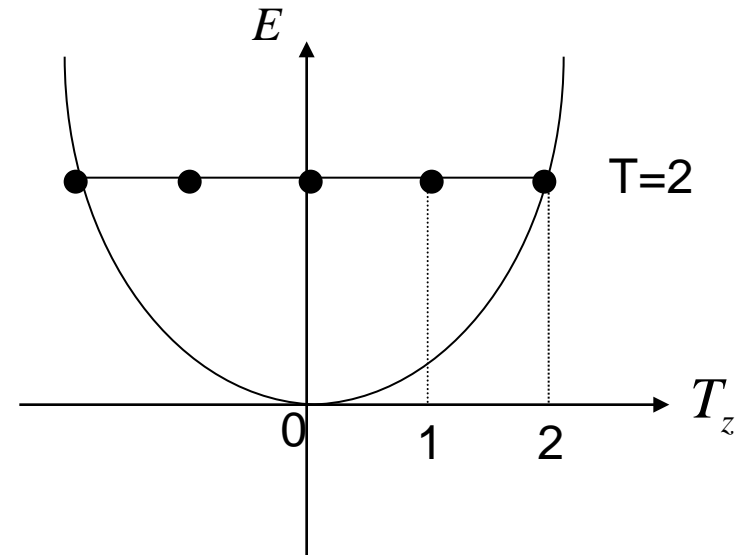


# Calculation for A=14 isobars

- w/ p-n mixing and no Coulomb
- w/ p-n mixing and Coulomb



Isobaric symmetry



**Figure 1-7** The level schemes for the nuclei with  $A = 14$  are based on the compilation by F. Ajzenberg-Selove and T. Lauritsen, *Nuclear Phys.* **11**, 1 (1959), on the results given by D. E. Alburger, A. Gallmann, J. B. Nelson, J. T. Sample, and E. K. Warburton, *Phys. Rev.* **148**, 1050 (1966), and on a private communication by G. Ball and J. Cerny (August, 1966). The relative energies represent atomic masses.

# Without Coulomb interaction

(Initial : 14C)

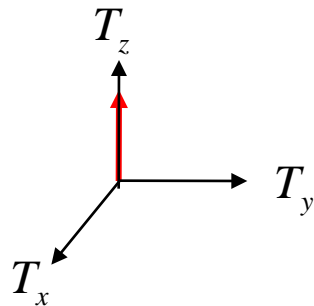
$(\theta, \varphi) = (0, 0)$

NO)	ENERGY	<T>
1)	<u>-38.419</u>	100
2)	-38.419	100
3)	-32.707	-100
4)	-32.707	-100
5)	-	-
6)	-	-
7)	⋮	⋮
8)	-	-
9)	-	-
10)	-	-
11)	-	-
12)	-	-
13)	-15.181	100
14)	-15.181	100

the same s. p energies

Total energy: -114.611699

$$\langle \hat{T}_z \rangle = 1$$



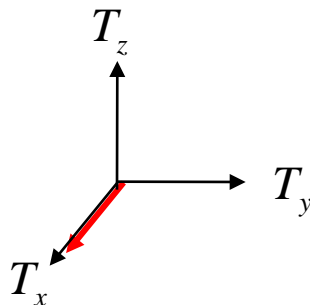
$(\theta, \varphi) = (90^\circ, 0)$

NO)	ENERGY	<T>
1)	<u>-38.419</u>	0
2)	-38.419	0
3)	-32.707	0
4)	-32.707	0
5)	-	-
6)	-	-
7)	⋮	⋮
8)	-	-
9)	-	-
10)	-	-
11)	-	-
12)	-	-
13)	-15.181	0
14)	-15.181	0

Total energy: -114.611699

$$\langle \hat{T}_z \rangle = 0$$

50% neutron & 50% proton

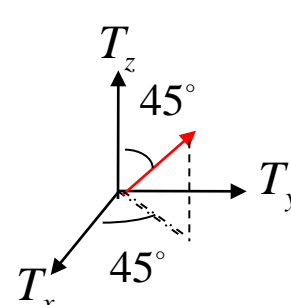


$(\theta, \varphi) = (45^\circ, 45^\circ)$

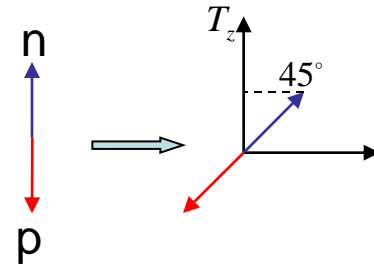
NO)	ENERGY	<T>
1)	<u>-38.419</u>	70.7
2)	-38.419	70.7
3)	32.707	-70.7
4)	-32.707	-70.7
5)	-	-
6)	-	-
7)	⋮	⋮
8)	-	-
9)	-	-
10)	-	-
11)	-	-
12)	-	-
13)	-15.181	70.7
14)	-15.181	70.7

Total energy: -114.611699

$$\langle \hat{T}_z \rangle = 0.707$$



$$\frac{|\vec{\lambda}|}{2} = 5.5$$



the same total energies

$$\langle T \rangle = \left\langle \frac{1}{2} \tau_z \right\rangle \times 200$$

- 100: pure n
- 100: pure p

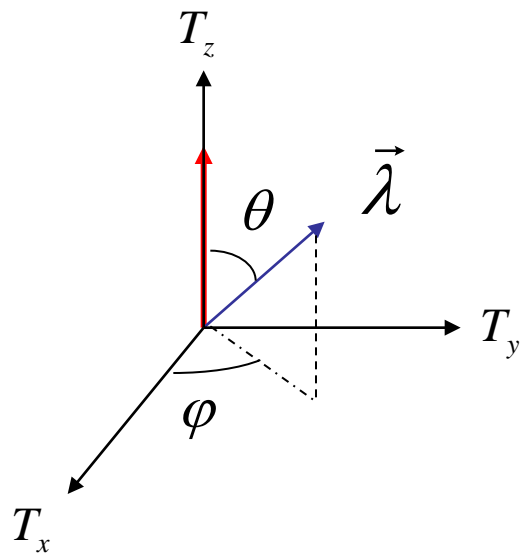
## With Coulomb interaction

$U^{Coulomb}(\tau_z)$  :violates isospin symmetry

The total energy is now dependent on  $T_z$

but independent of  $T_x$  and  $T_y$

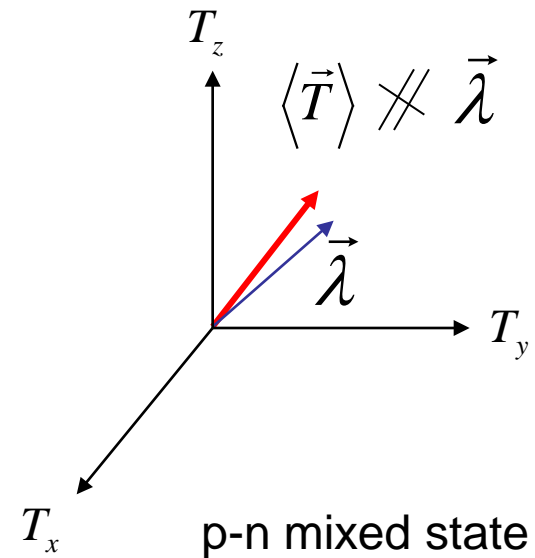
Initial state:



HF state w/o p-n mixing

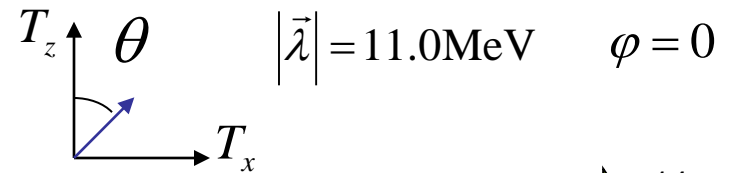
$$-\vec{\lambda} \cdot \hat{T}$$

final state:



With Coulomb, larger  $\langle T_z \rangle$  is favored

# With Coulomb interaction



$\theta = 0^\circ$   $\rightarrow$   $^{14}\text{C}$

$\theta = 45^\circ$

$\theta = 180^\circ$   $\rightarrow$   $^{14}\text{O}$

single-particle energy:

NO)	ENERGY	<Tz>
1)	<u>-38.346</u>	100
2)	<u>-38.346</u>	100
3)	-29.620	-100
4)	-29.620	-100
5)	-22.000	100
6)	-22.000	100
7)	.	.
8)	.	.
9)	.	.
10)	.	.
11)	.	.
12)	.	.
13)	.	.
14)	.	.

Single-particle energy:

NO)	ENERGY	<Tz>
1)	<u>-37.980</u>	82.0
2)	<u>-37.980</u>	82.0
3)	-29.880	-82.0
4)	-29.880	-82.0
5)	-21.666	80.7
6)	-21.666	80.7
7)	.	.
8)	.	.
9)	.	.
10)	.	.
11)	.	.
12)	.	.
13)	.	.
14)	.	.

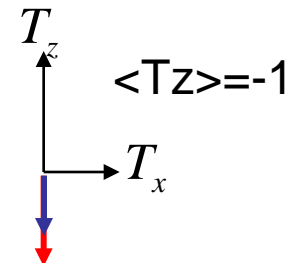
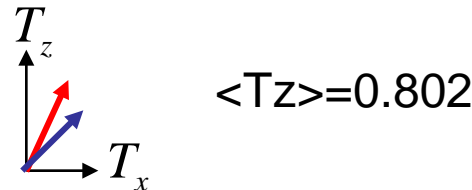
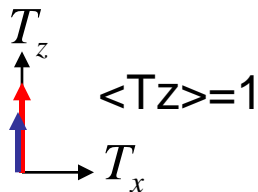
single-particle energy:

NO)	ENERGY	<Tz>
1)	<u>-34.362</u>	-100
2)	<u>-34.362</u>	-100
3)	-32.527	100
4)	-32.527	100
5)	-18.41	-100
6)	-18.41	-100
7)	.	.
8)	.	.
9)	.	.
10)	.	.
11)	.	.
12)	.	.
13)	.	.
14)	.	.

Total energy: -106.68

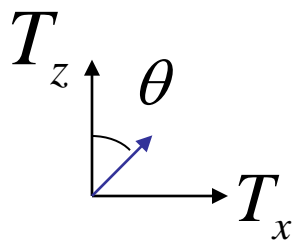
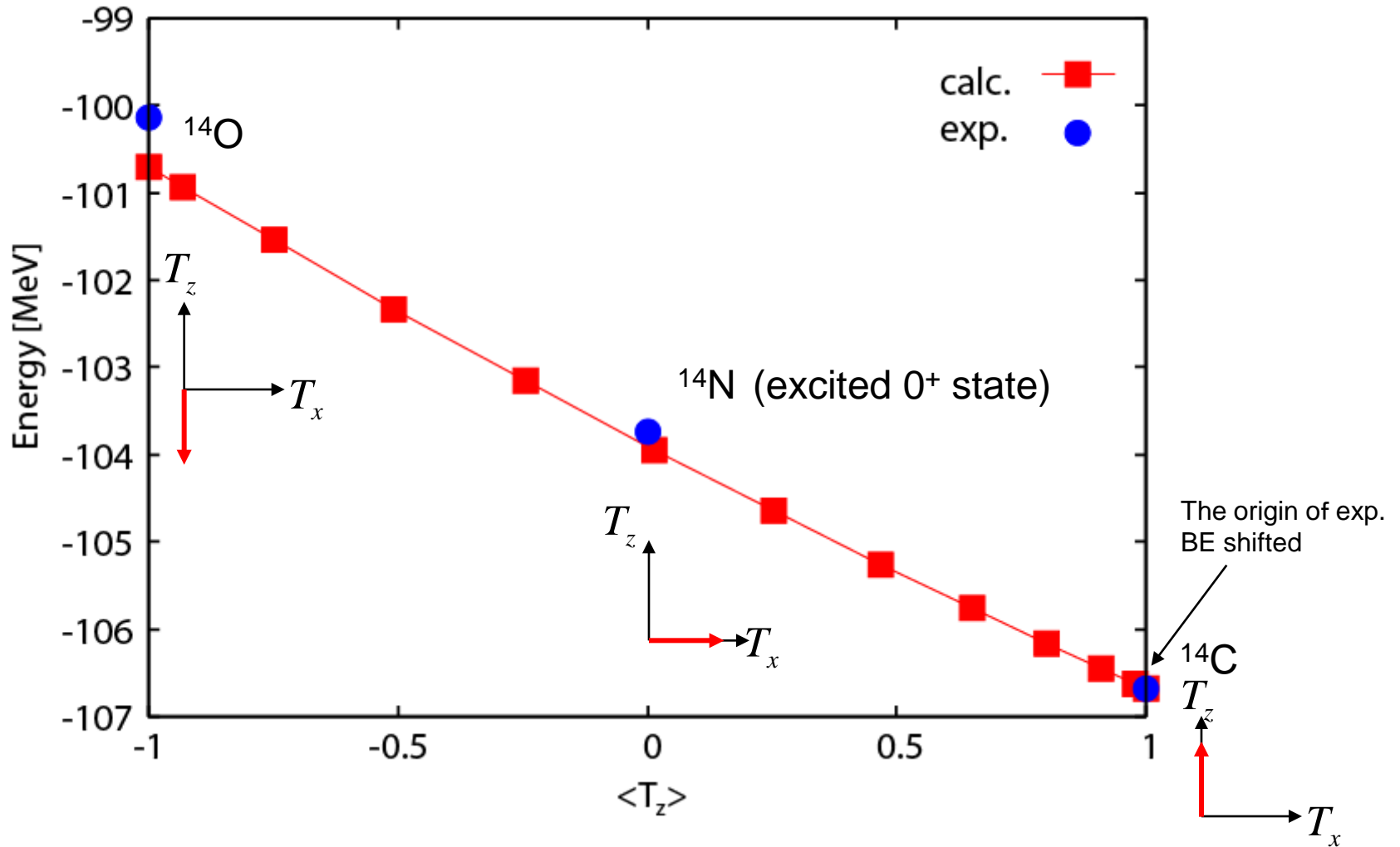
Total energy: -106.16

Total energy: -100.70



- Total and s. p. energies depend on  $\langle Tz \rangle$
- Total isospin and  $\vec{\lambda}$  are not parallel for p-n mixed states
- No p-n mixing for  $\theta = 0^\circ$  and  $\theta = 180^\circ$   
(Neither Coulomb nor isocranking term contains  $T_x$  and  $T_y$ .)

*Tz dep. of the total energy and comparison with data*

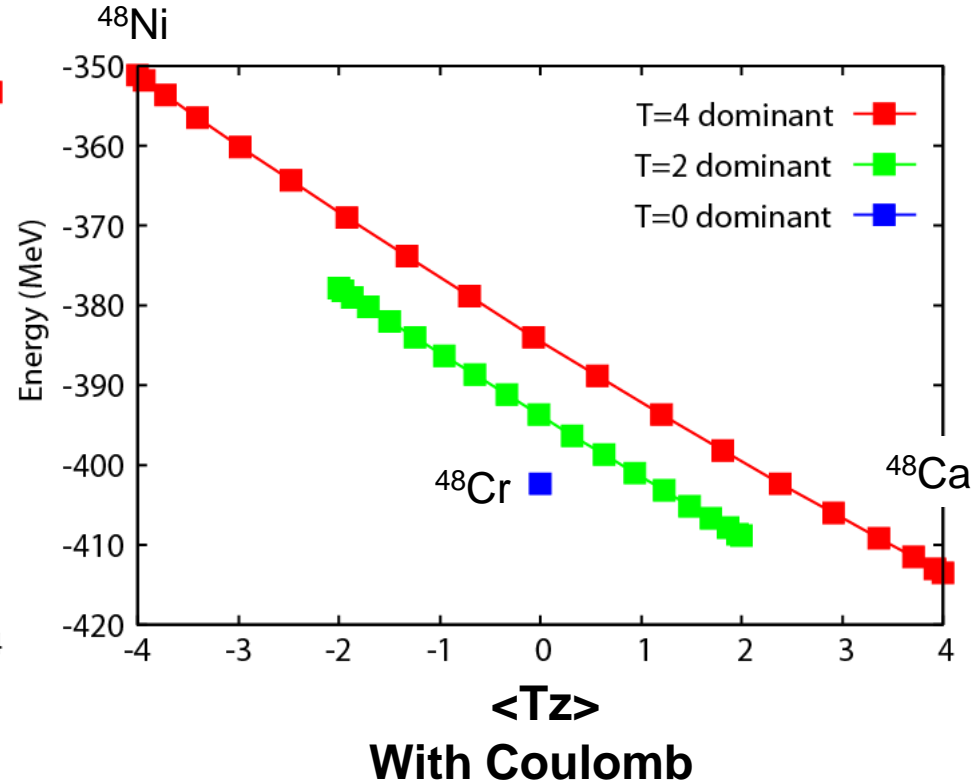
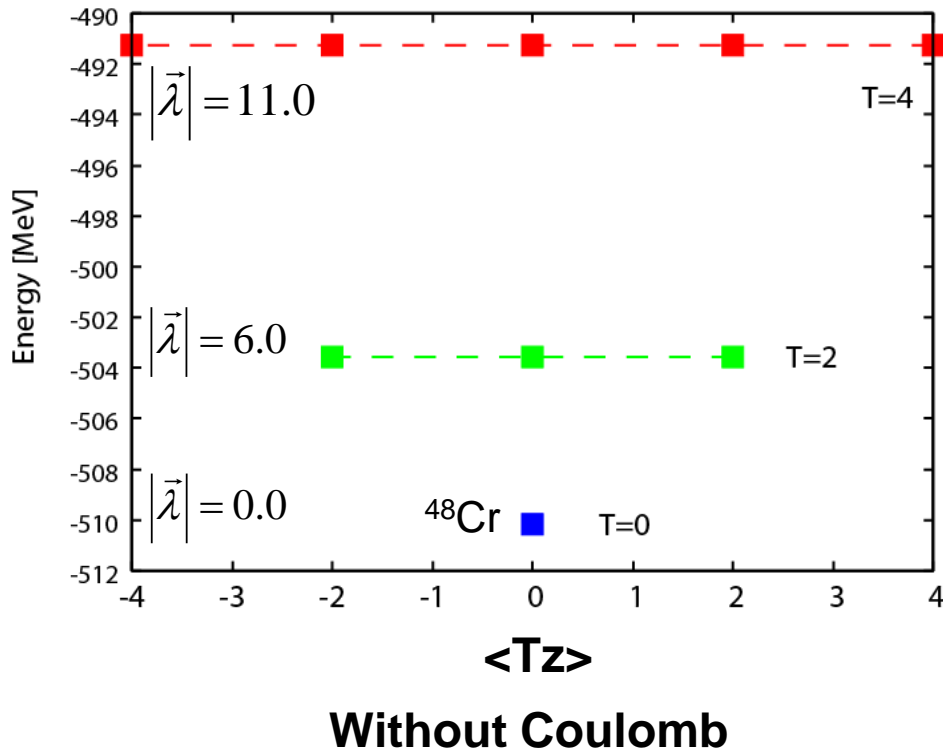


exp.: binding energy  
(+excitation energy for  $^{14}\text{N}$ )

calc.: calculated for  
every  $15^\circ$  of  $\theta$  from  $0$  to  $180^\circ$

# Result for A=48 isobars

Initial :  $^{48}\text{Cr}(T_z=0, T\sim 0)$



## Without Coulomb

- ◇ Increase the size of isofrequency  $|\vec{\lambda}|$  to make high-isospin states

## With Coulomb

- ◇ Tune the size of lambda depending on the tilting angle  $\theta$
- ◇ Diabatic blocking with isospin to avoid oscillatory (ping-pong) divergence

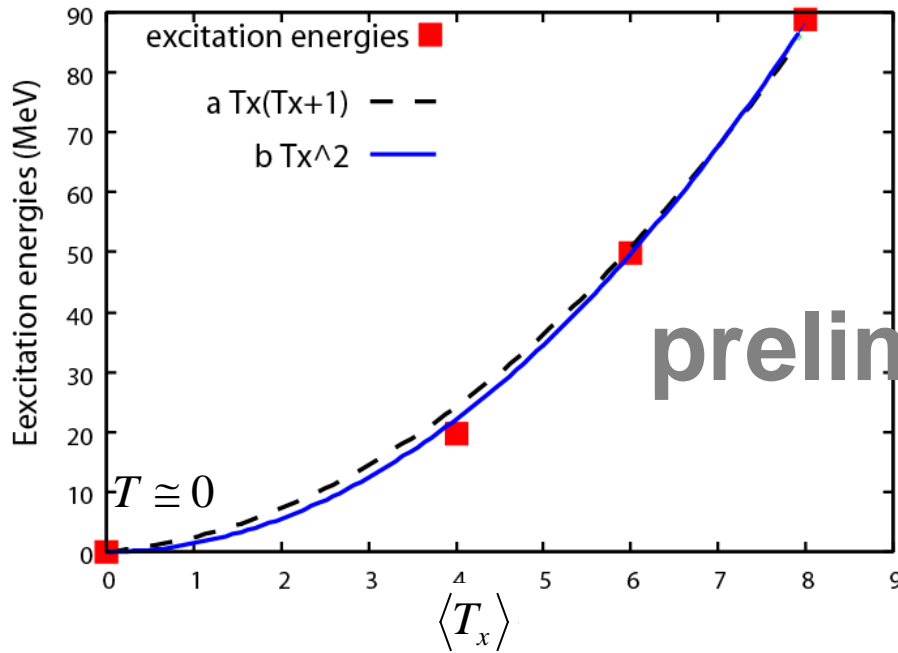
# Constrained HF with Augmented Lagrange method

$$E' = E - \vec{\lambda} \cdot \hat{T} + C \left( \hat{T} - \bar{T} \right)^2$$

A. Staszczak, Eur. Phys. J. A **46**, 85–90 (2010)

## Excitation energies for $^{48}\text{Cr}(T_z=0)$

constraints  $T_z=0$  and  $T_x=0,2,4,6,\dots$



--> nuclear symmetry energy

$$a = 1.20956 \text{ (MeV)}$$

$$b = 1.38078 \text{ (MeV)}$$

Sum of squared residuals :

$$a * T_x * (T_x + 1) \text{ fit} : 24.2$$

$$b * T_x^2 \text{ fit} : 6.1$$

preliminary

$\bar{T}_x$	$ \langle \hat{T}_x \rangle - \bar{T}_x $	$\bar{T}_z$	$ \langle \hat{T}_z \rangle - \bar{T}_z $	Energy
2		0		Not yet
4	3.6E-05	0	<1.0E-08	-390.06
6	9.8E-04	0	5.7E-06	-359.76
8	9.4E-04	0	3.1E-06	-320.89

## Summary

We have developed a code for the DFT calculations with

- ✓ proton-neutron mixing at the Hartree-Fock level
- ✓ diabatic blocking method using isospin
- ✓ constraints on isospin with augmented Lagrange method

and performed test calculations for  $A=14$  & 48 systems

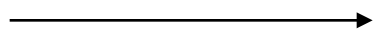
## Ongoing

- ◇ Isospin projection to remove spurious isospin mixing

W. Satuła et al., PRC 81, 054310 (2010).

## Future

- ◇ Proton-neutron pairing ( $T=0$  &  $T=1$ ; non-rotating & rotating)
- ◇ Charge exchange reaction in neutron-rich nuclei (QRPA calculation)



A very wide applicability expected